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A Hybrid Model for Multiscale Laser Plasma Simulations with Detailed Collisional Physics

AFOSR Plasma and Electroenergetics Review Meeting
29-30 November 2016

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- A. Karagozian (UCLA)

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Outline

- Goals
- Review of Past Work
- Argon Collisional-Radiative Complexity Reduction Validation
- Non-Maxwellian CR
- Phase-accurate Multiscale Particle Push

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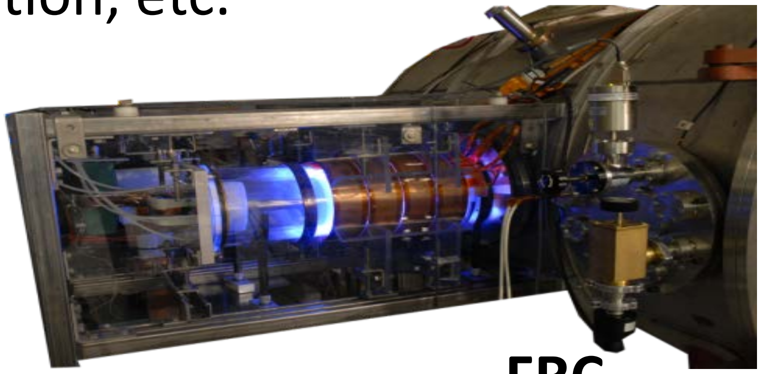
Goals

- Utilize hybridization techniques to produce accurate and efficient plasma simulations that spans many orders of magnitude in both space and time.
- Capture complex physics: excitation/ionization, transport, radiation, etc.
- Consistent collision operator across different levels of fidelity.

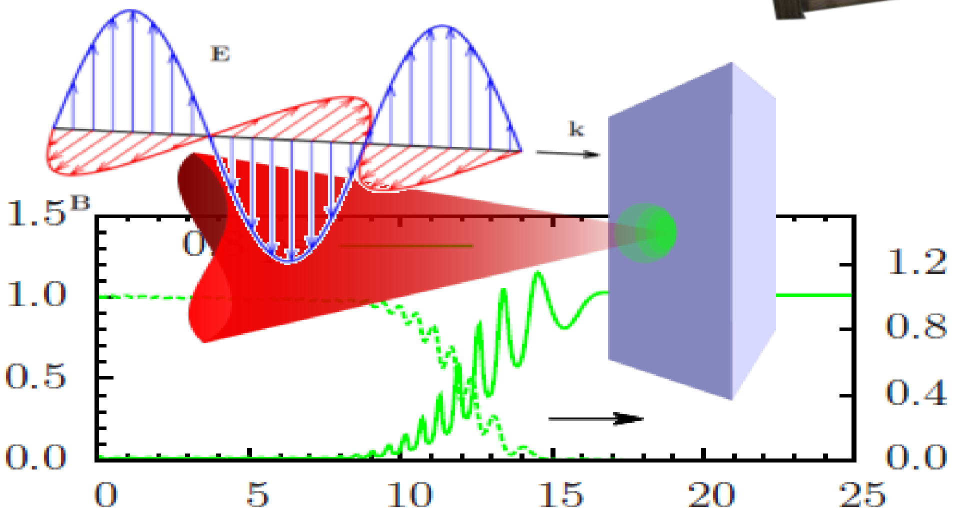


FRC

<u>Current Focus:</u>

- Generalization of collisional-radiative kinetics with level grouping
- General Hybridization techniques
- Focus on each solver before hybridization
- Special attention to low density low energy conditions

Laser Plasma Interaction



RQRS M&S Group

- **Government**
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  - Dr. Justin Koo (Flight Support, Group Lead)
  - Dr. Rob Martin (FRC)
- **Onsite Contractors (ERC inc.)**
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  - Dr. Jun Araki (Flight Support, PIC)
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- **Summer Students**
  - Astrid Raisanen
    - PhD UofM; Vlasov HET
  - Daniel Crews
    - M.S. Washington; Collisionless Shock for V&V
  - Kari Kawashima
    - B.S. UCLA; SM/MURF beta tester
- **Previous**
  - Dr. Hai Le (LPI; now at Livermore)
  - Dr. Artan Qerushi (FRC now at Lockheed)

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Summary of Past Work

Maxwellian Inelastic Collisions

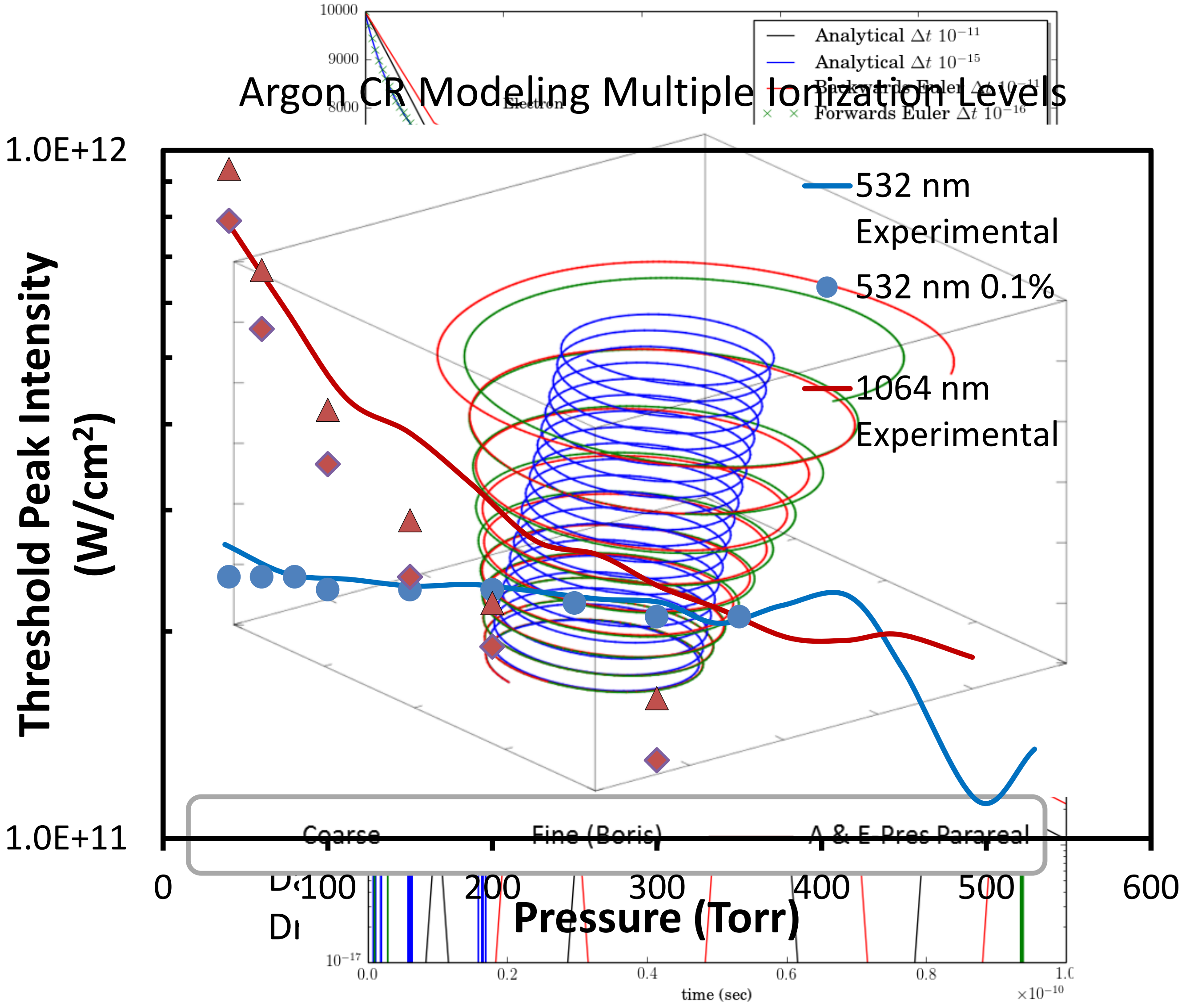
- Detailed CR model for multiple ionization stages
- Validation against experimental data
- Nonequilibrium radiation transport: coupling with a collisional-radiative model
- Inelastic collisions in a MF plasma: enhanced thermochemical kinetics.

Multiscale Hybridization

- A time-parallel/multiscale method with energy preservation

Analytical BGK

- Conservative even for large mass ratios
- Conservation are independent of collisional frequencies



Collisional Radiative (CR) Overview

Updates

- Expanded complexity reduction to include multiple ionization levels
- Adaptive integration technique -> fixes rate calculation for higher electron temperature
- Investigate grouping sensitivity
- Linked with LANL database for Argon cross sections and atomic level information
- Algorithms not hard coded for Argon.

Levels of Complexity

- Full rates (LANL)
- Cutoff nearly ionized levels
- Grouping Strategies
  - Uniform
  - Boltzmann
  - QSS (Boltzmann and Planck equilibrium)
- Group Selection
  - Electron configuration (no splitting information)
  - Highly excited states
  - Analysis of full run
  - Numerical optimization

CR Governing Equations

$$\left(\frac{df_e(\varepsilon,t)}{dt}\right)_{\text{coll,ex/dex}} = -\sum_{m>n} N_n(f_e(\varepsilon_0))\left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)\sigma^{e,\uparrow}_{(m|n)}(\varepsilon_0)$$
$$+\sum_{m>n} N_m(f_e(\varepsilon_1))\left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\sigma^{e,\downarrow}_{(n|m)}(\varepsilon_1)$$
$$+\sum_{m<n} N_m(f_e(\varepsilon_1))\left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\sigma^{e,\uparrow}_{(n|m)}(\varepsilon_1)$$
$$-\sum_{m>n} N_n(f_e(\varepsilon_0))\left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)\sigma^{e,\downarrow}_{(m|n)}(\varepsilon_0)$$

$$\left(\frac{df_e(\varepsilon,t)}{dt}\right)_{\text{coll,i/r}} =$$
$$-\sum_n N_n(f_e(\varepsilon))\left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)\sigma^{e,\uparrow}_{(+|n)}(\varepsilon_0)$$
$$+N_+\int_{\varepsilon_1}\int_{\varepsilon_2}(f_e(\varepsilon_1))(f_e(\varepsilon_2))\left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right)\left(\frac{\partial^2}{\partial\varepsilon_1\partial\varepsilon_2}\sigma^{e,\downarrow}_{(n|+)}(\varepsilon_1,\varepsilon_2;\varepsilon_0)\right)d\varepsilon_1 d\varepsilon_2$$
$$-N_+(f_e(\varepsilon_2))\left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right)\int_{\varepsilon_0}\int_{\varepsilon_1}(f_e(\varepsilon_1))\left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\left(\frac{\partial^2}{\partial\varepsilon_1\partial\varepsilon_2}\sigma^{e,\downarrow}_{(n|+)}(\varepsilon_1,\varepsilon_2;\varepsilon_0)\right)d\varepsilon_1 d\varepsilon_0$$
$$+\sum_n N_n\int_{\varepsilon_1}\int_{\varepsilon_0}\left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)(f_e(\varepsilon_0))\left(\frac{\partial^2}{\partial\varepsilon_1\partial\varepsilon_2}\sigma^{e,\uparrow}_{(+|n)}(\varepsilon_2;\varepsilon_0,\varepsilon_1)\right)d\varepsilon_0 d\varepsilon_1$$

$$\left(\frac{dN_n(t)}{dt}\right)_{\text{coll,ex/dex}} = -\sum_{m>n} N_n\int_{\varepsilon_0}(f_e(\varepsilon_0))\left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)\sigma^{e,\uparrow}_{(m|n)}(\varepsilon_0)d\varepsilon_0$$
$$+\sum_{m>n} N_m\int_{\varepsilon_1}(f_e(\varepsilon_1))\left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\sigma^{e,\downarrow}_{(n|m)}(\varepsilon_1)d\varepsilon_1$$
$$+\sum_{m<n} N_m\int_{\varepsilon_1}(f_e(\varepsilon_1))\left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\sigma^{e,\uparrow}_{(n|m)}(\varepsilon_1)d\varepsilon_1$$
$$-\sum_{m<n} N_n\int_{\varepsilon_0}(f_e(\varepsilon_0))\left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)\sigma^{e,\downarrow}_{(m|n)}(\varepsilon_0)d\varepsilon_0$$

$$\left(\frac{dN_n(t)}{dt}\right)_{\text{coll,i/r}} =$$
$$-N_n\int_{\varepsilon_0}(f_e(\varepsilon_0))\left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)\sigma^{e,\uparrow}_{(+|n)}(\varepsilon_0)d\varepsilon_0$$
$$+N_+\int_{\varepsilon_0}\int_{\varepsilon_1}\int_{\varepsilon_2}(f_e(\varepsilon_1))(f_e(\varepsilon_2))\left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right)\left(\frac{\partial^2}{\partial\varepsilon_1\partial\varepsilon_2}\sigma^{e,\downarrow}_{(n|+)}(\varepsilon_1,\varepsilon_2;\varepsilon_0)\right)d\varepsilon_1 d\varepsilon_2$$

CR Governing Equations cont.

- **Current Assumptions**
  - Electron dominated collisions
  - δ function for ion distribution
  - Maxwellian electrons
- **Current Model Includes**
  - Multiple ionization levels
  - Excitation/de-excitation
  - Ionization/recombination
  - Multi-photon ionization and inverse Bermsstrahlung
  - Radiation losses via, Bound-Bound and Bound-Free

*previous included

$$\frac{dn_n^{+k}}{dt} =$$

$$-\sum_{m>n}\alpha_{(m|n)}^{+k,e}N_eN_{+k,n}+\sum_{m>n}\beta_{(n|m)}^{+k,e}N_eN_{+k,m}+\sum_{m>n}A_{(n|m)}^{+k}N_{+k,m}$$

$$+\sum_{m<n}\alpha_{(n|m)}^{+k,e}N_eN_{+k,m}-\sum_{m<n}\beta_{(m|n)}^{+k,e}N_eN_{+k,n}-\sum_{m<n}A_{(m|n)}^{+k}N_{+k,n}$$

$$-\sum_{j}\alpha_{(+,j|n)}^{+k,e}N_eN_{+k,n}+\sum_{j}\beta_{(n|+,j)}^{+k,e}N_{+(k+1),j}N_e^2$$

$$\alpha_{(m|n)}^{e} = \int_{E_{nm}}^{\infty}\sigma_{nm}^{e}(\varepsilon)v_e f(v_e)dv_e$$

$$\beta_{(n|m)}^{e} = \frac{n^2}{m^2}e^{+x_{nm}}\alpha_{(m|n)} \qquad A_{(n|m)} = \left(\frac{8\pi^2e^2}{m_ec^3}\right)\frac{g_n}{g_m}f_{nm}$$

CR Grouping Techniques

Uniform

- Solely conserves number density
- Weights each level according to level degeneracy within group

Conserved Variable:

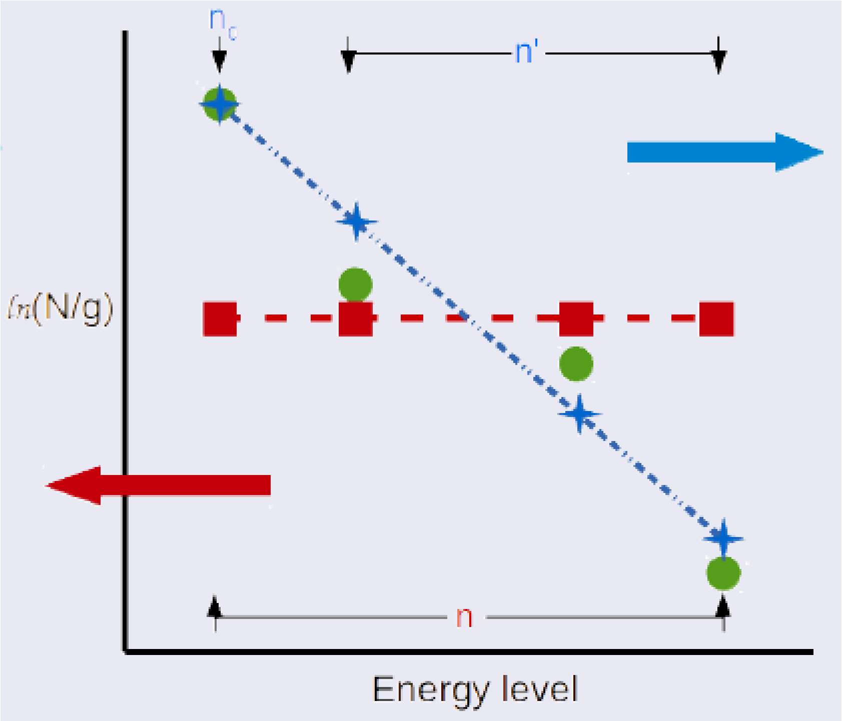
$$\tilde{N}_n = \sum_{i\in n} N_i$$

Effective rate:

$$\tilde{\alpha}_{(m|n)} = \sum_{i\in n} \frac{g_i}{g_n} \sum_{j\in m} \alpha_{(j|i)}$$

$$\frac{dN_n}{dt} = N_e\left[\sum_{m>n} \alpha_{(m|n)} N_n + \sum_{m<n} \beta_{(m|n)} N_n\right] + \cdots$$

$$\frac{d\tilde{N}_n}{dt} = N_e \tilde{N}_n\left[\sum_{m>n} \tilde{\alpha}_{(m|n)} + \sum_{m<n} \tilde{\beta}_{(m|n)}\right] + \cdots$$



Boltzmann

- Conserves number density
- Preserves energy in groups through group temperature description

Conserved Variable:

$$N_{n_0} \& N'_n = \frac{N_{n_0}}{g_{n_0}} \sum_{i\in n} g_i e_i^{-\Delta E_i/T_n}$$

Effective rate:

$$\tilde{\alpha}_{(m'|n')} = \sum_{i\in n} \frac{g_i e^{-\Delta E_i/T_n}}{Z'_n} \sum_{j\in m'} \alpha_{(j|i)}$$

Complexity Reduction for Argon

Full Lines (LANL)

- Based on quantum calculations with corrections for low temperature

NIST Cutoff

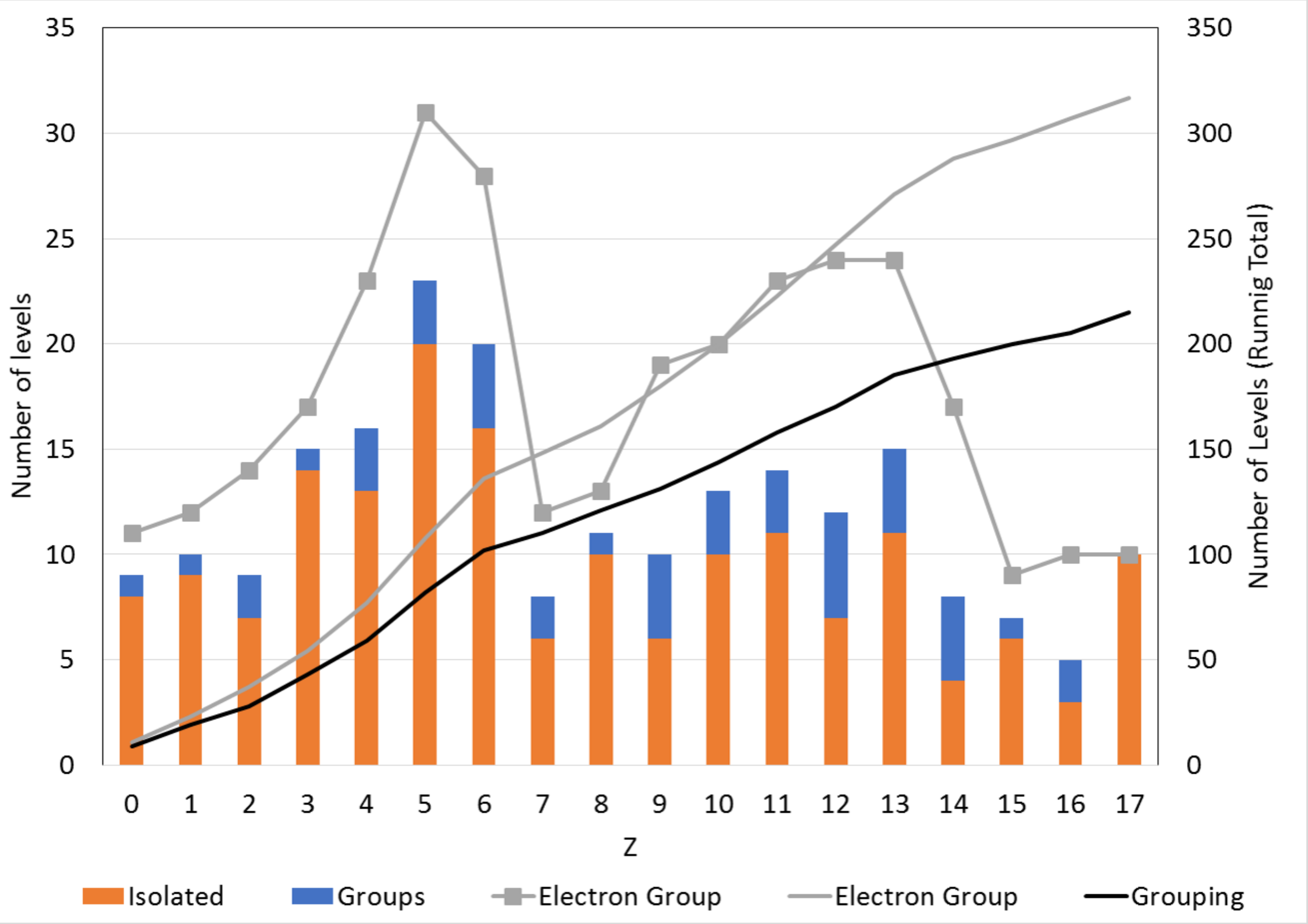
- Starts with LANL and assumes higher excited states are ionized
- Cutoff experimentally determined
- 2-3x reduction

Electron Configuration

- Groups based on electron configuration
- Uses uniform grouping
- 10-15x reduction over NIST

Grouping

- Boltzmann or Uniform grouping
- Saves 20-30% over Electron Splitting
- Case by case basis



Argon Level Grouping Isothermal Test Setup

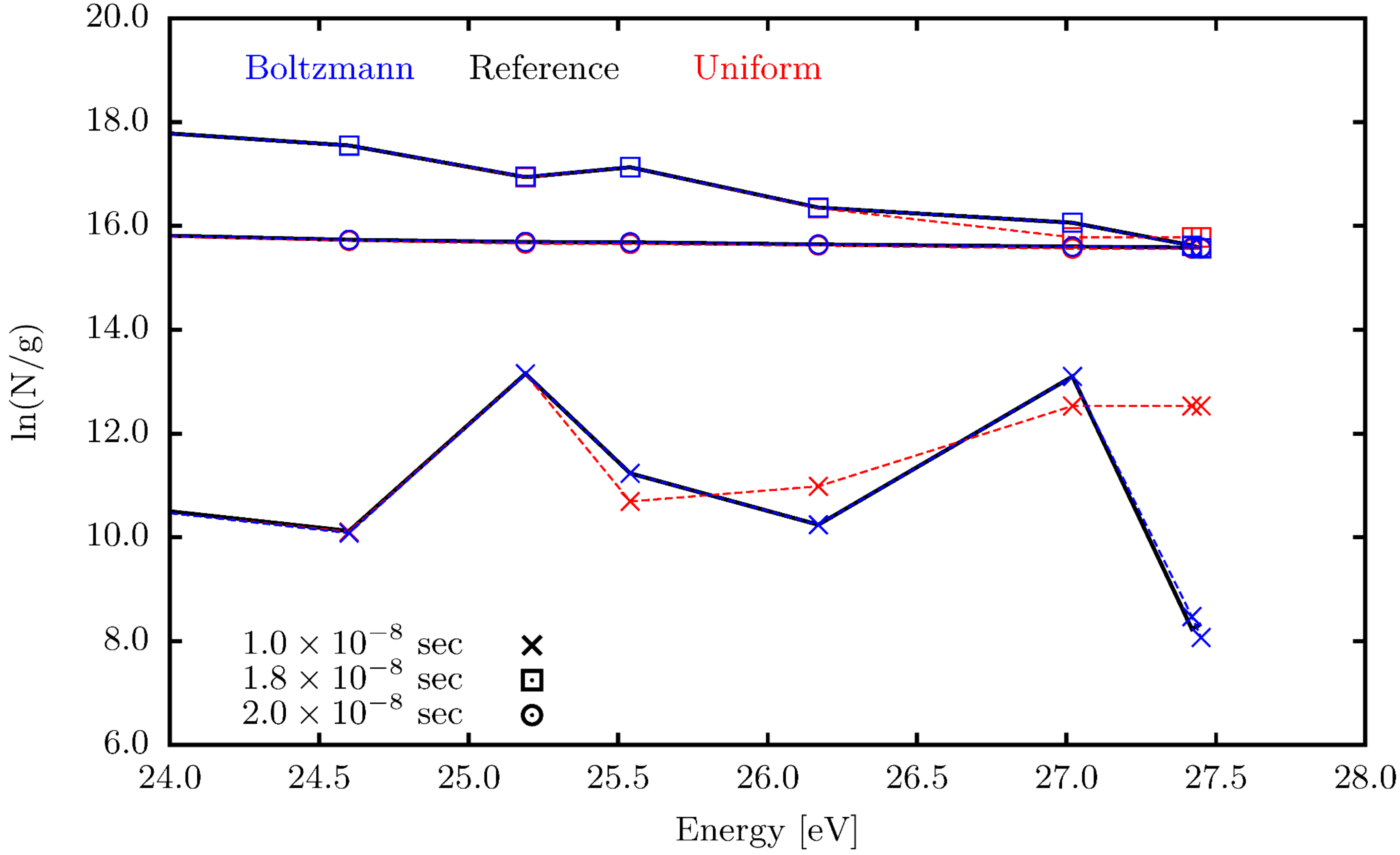
Simulation Setup

- Pressure: 4.22 Torr (5.55×10^{-3} atm)
- Ion Temperature: 0.035 eV
- Atomic Density: 10^{20} $1/m^3$
- Ionization fraction: 10^{-13}
- Electron Temperature: 10 & 100 eV
- $t = [0, 10^6]$ seconds

Groupings

- NIST cutoff with electron grouping
- NIST cutoff with electron grouping and Boltzmann grouping
- NIST cutoff with electron grouping and Uniform grouping

Argon Level Grouping Isothermal Test
Electron Temperature 10 eV



Argon +1

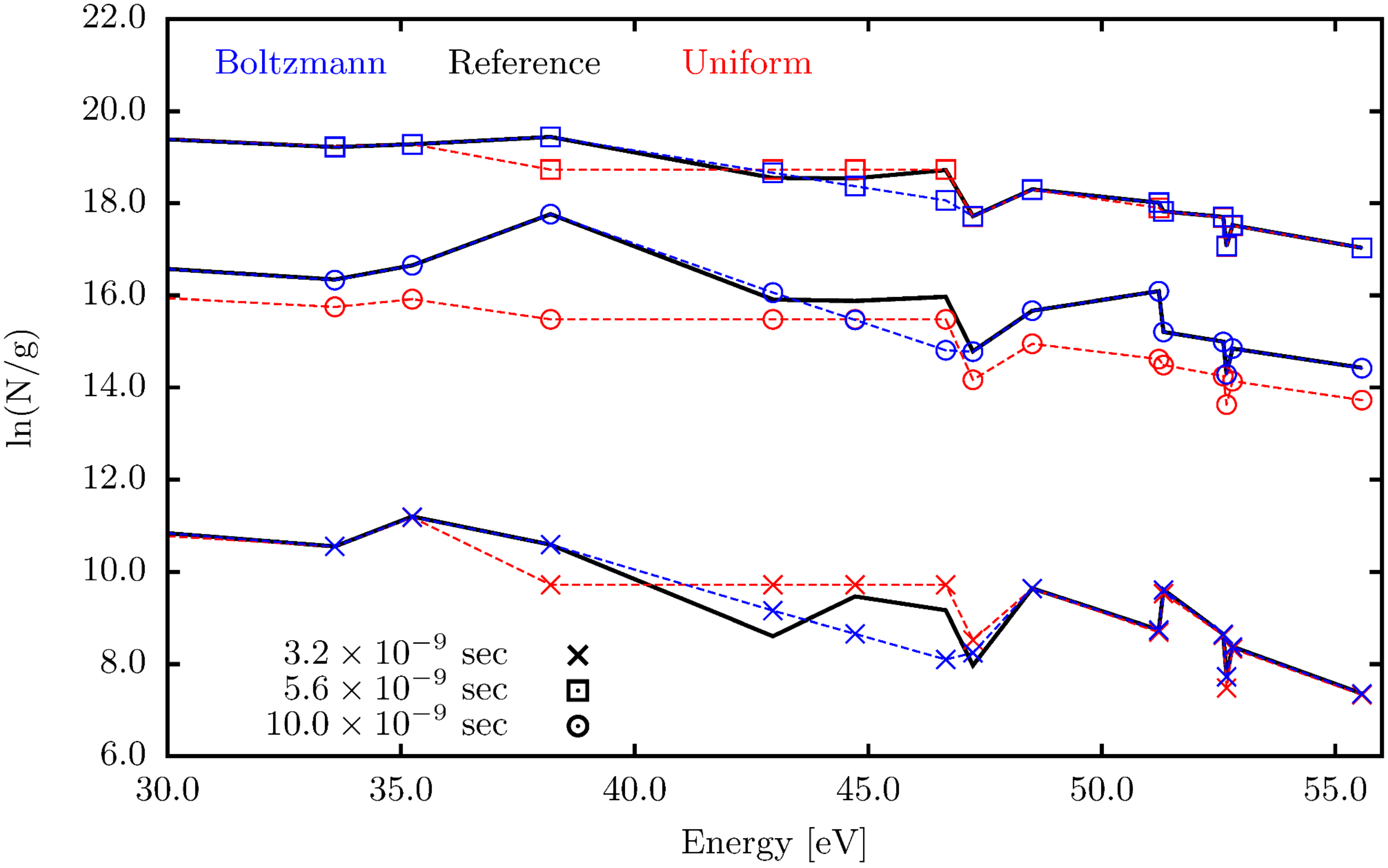
12 electron configurations

9 Isolates states

1 group with 3 states

Uniform group propagates errors to isolated states

Argon Level Grouping Isothermal Test
Electron Temperature 100 eV



Argon +3

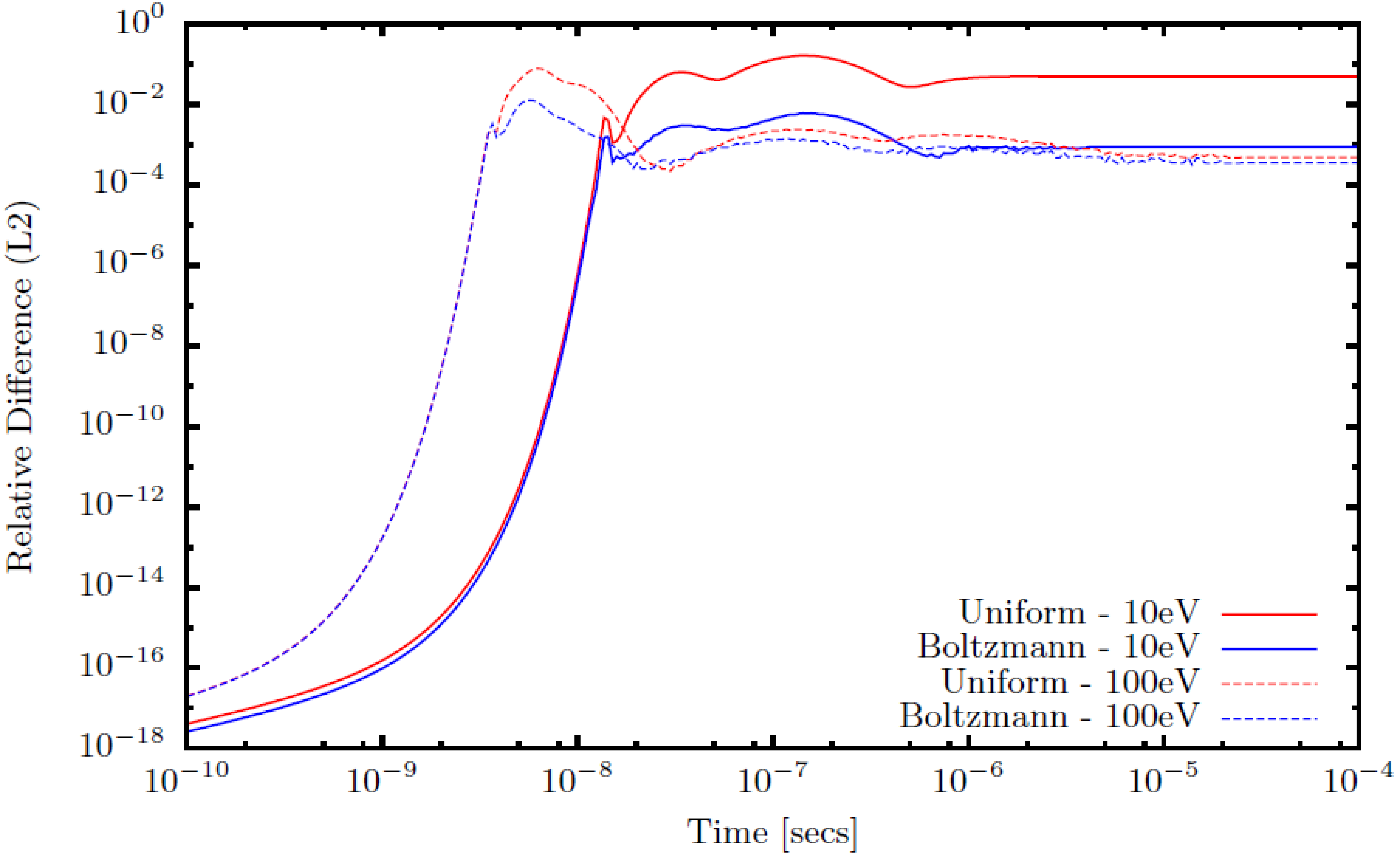
17 electron configurations

14 Isolates states

1 group with 3 states

Uniform groups propagates errors to isolated states

Argon Level Grouping Isothermal Test Error



ODE Solver tolerance
Relative error 1^{-4}
Absolute error 1
~1200 Radau5 time steps
dt increases exponentially

Solution improves if either tolerance is decreased but at the expense of computational time. E.g. relative error 10^{-6} -> computational time triples

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Non-Maxwellian Electrons CR - Ions
(Preliminary)

- **Current Assumptions**
  - Electron dominated collisions
  - Single ionization level
  - Isotropic EEDF
  - δ function for ion distribution
- **Current Model Includes**
  - Elastic electron collisions
  - Excitation/de-excitation
  - Ionization/recombination

$$\left(\frac{dN_n(t)}{dt}\right)_{\mathrm{coll,ex/dex}} = -\sum_{m>n} N_n \boxed{\int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma^{e,\uparrow}_{(m|n)}(\varepsilon_0) d\varepsilon_0}$$
$$+\sum_{m>n} N_m \boxed{\int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma^{e,\downarrow}_{(n|m)}(\varepsilon_1) d\varepsilon_1}$$
$$+\sum_{m<n} N_m \boxed{\int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma^{e,\uparrow}_{(n|m)}(\varepsilon_1) d\varepsilon_1}$$
$$-\sum_{m<n} N_n \boxed{\int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma^{e,\downarrow}_{(m|n)}(\varepsilon_0) d\varepsilon_0}$$

$$\left(\frac{dN_n(t)}{dt}\right)_{\mathrm{coll,i/r}} =$$
$$-N_n \boxed{\int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma^{e,\uparrow}_{(+|n)}(\varepsilon_0) d\varepsilon_0}$$
$$+N_+ \boxed{\int_{\varepsilon_0} \int_{\varepsilon_1} \int_{\varepsilon_2} (f_e(\varepsilon_1))(f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right) \left(\frac{\partial^2}{\partial\varepsilon_1 \partial\varepsilon_2} \sigma^{e,\downarrow}_{(n|+)}(\varepsilon_1, \varepsilon_2; \varepsilon_0)\right) d\varepsilon_1 d\varepsilon_2}$$

Non-Maxwellian Electrons CR - Electrons
(Preliminary)

- **Current Assumptions**
  - Electron dominated collisions
  - Single ionization level
  - Isotropic EEDF
  - δ function for ion distribution
- **Current Model Includes**
  - Elastic electron collisions
  - Excitation/de-excitation
  - Ionization/recombination

$$\left(\frac{df_e(\varepsilon,t)}{dt}\right)_{\mathrm{coll,ex/dex}} = -\sum_{m>n} N_n(f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma^{e,\uparrow}_{(m|n)}(\varepsilon_0)$$
$$+\sum_{m>n} N_m(f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma^{e,\downarrow}_{(n|m)}(\varepsilon_1)$$
$$+\sum_{m<n} N_m(f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma^{e,\uparrow}_{(n|m)}(\varepsilon_1)$$
$$-\sum_{m>n} N_n(f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma^{e,\downarrow}_{(m|n)}(\varepsilon_0)$$

$$\left(\frac{df_e(\varepsilon,t)}{dt}\right)_{\mathrm{coll,i/r}} =$$
$$-\sum_n N_n(f_e(\varepsilon)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma^{e,\uparrow}_{(+|n)}(\varepsilon_0)$$
$$+N_+ \boxed{\int_{\varepsilon_1}\int_{\varepsilon_2} (f_e(\varepsilon_1))(f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right)\left(\frac{\partial^2}{\partial\varepsilon_1\partial\varepsilon_2}\sigma^{e,\downarrow}_{(n|+)}(\varepsilon_1,\varepsilon_2;\varepsilon_0)\right) d\varepsilon_1 d\varepsilon_2}$$
$$-N_+(f_e(\varepsilon_2))\left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right) \boxed{\int_{\varepsilon_0}\int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right)\left(\frac{\partial^2}{\partial\varepsilon_1\partial\varepsilon_2}\sigma^{e,\downarrow}_{(n|+)}(\varepsilon_1,\varepsilon_2;\varepsilon_0)\right) d\varepsilon_1 d\varepsilon_0}$$
$$+\sum_n N_n \boxed{\int_{\varepsilon_1}\int_{\varepsilon_0} \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right)(f_e(\varepsilon_0))\left(\frac{\partial^2}{\partial\varepsilon_1\partial\varepsilon_2}\sigma^{e,\uparrow}_{(+|n)}(\varepsilon_2;\varepsilon_0,\varepsilon_1)\right) d\varepsilon_0 d\varepsilon_1}$$

$$\left(\frac{df_e(\varepsilon,t)}{dt}\right)_{\mathrm{elastic}} = \nu_{ee}(F_e - f_e) + \nu_{ei}(F_{ei} - f_e)$$

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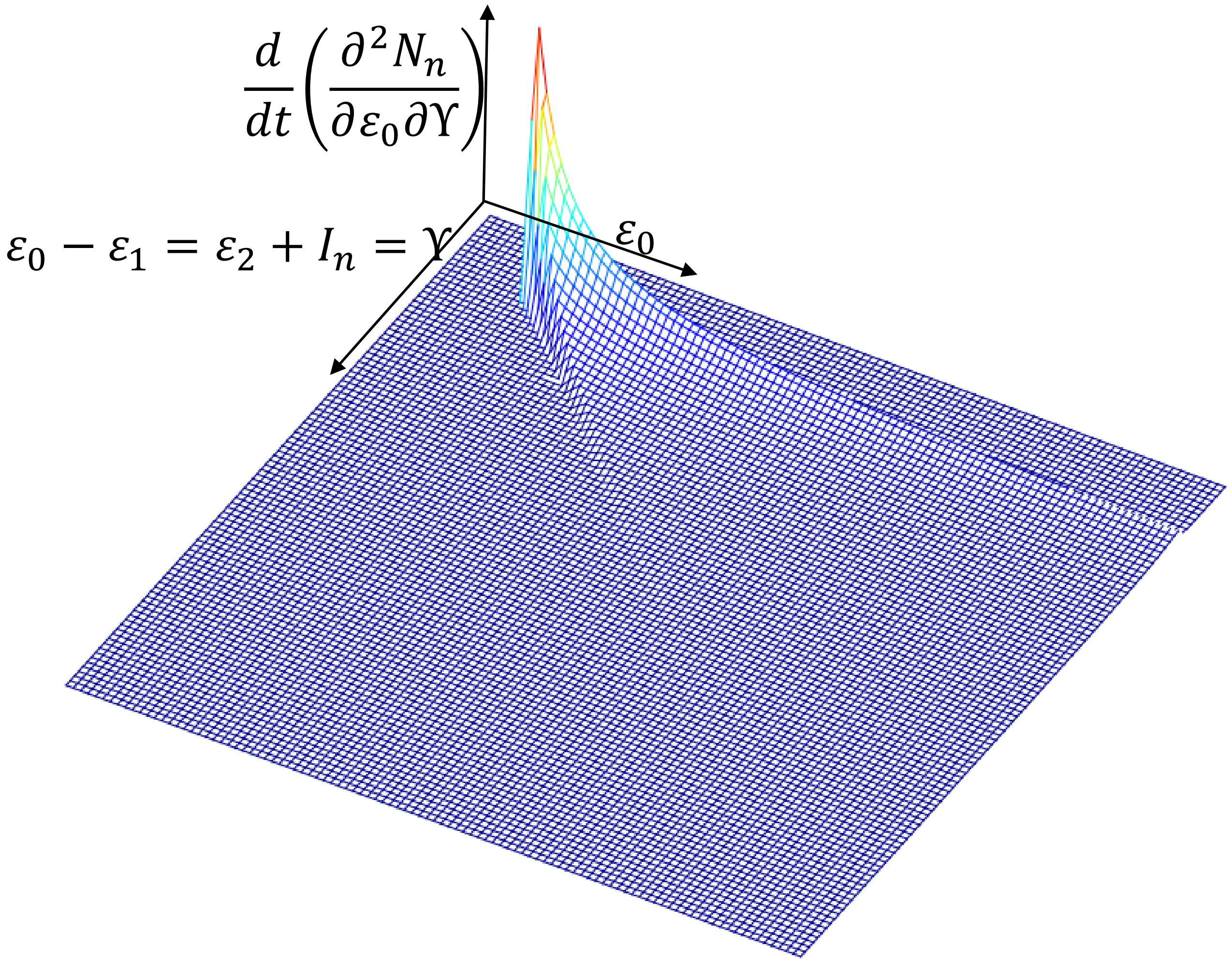
Non-Maxwellian CR Numerical Challenges

- **Long complex CR formulas**
- **Stiff equations**
- **Range of scales**
- **Boundary conditions**
- **Multi-dimensional integrations**



- Hydrogen recombination example:
- $e_0 + H_n \leftarrow e_1 + e_2 + H_+$
- Energy equation in terms of the electron's kinetic energies, ε, and ionization energy I_n.
- $\varepsilon_0 = \varepsilon_1 + \varepsilon_2 + I_n$
- Evaluating the effect of recombination on a single species of hydrogen requires the evaluation of a 2D integral.

Hybridization Techniques

- Solve ODE/PDE with a coarse "C" solver and fine "F" solver
- Coarse propagates less information and is more computationally efficient
- Fine propagates more information and is more accurate
- User defined coarse error function $h(u), 0 \leq h \leq 1$
- when h=0 coarse is accurate
- Q compression operator
- R reconstruction operator
- h, ε, Q, & R, are problem dependent

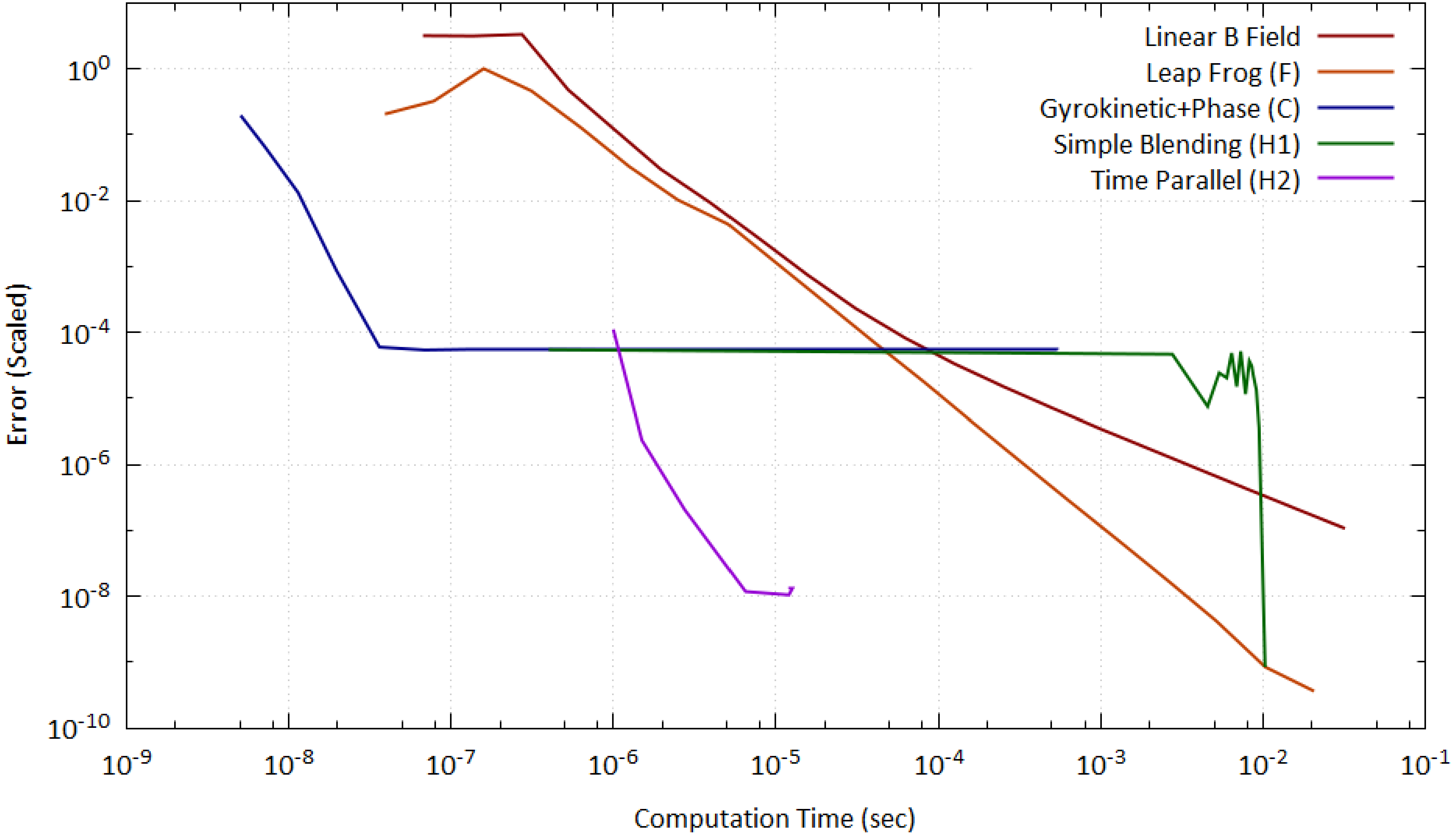
Simpler hybrid (H) method

$$H1_{[t+dt,t]} = \begin{cases} C_{[t+dt,t]}\big(Q(\text{if needed})\big) & \text{if } \; h \leq \epsilon \\ F_{[t+dt,t]}\big(R(\text{if needed})\big) & \text{if } \; h > \epsilon \end{cases}$$

More complex time parallel (TP) method

$$H2_{[Jdt,0]}(u(0)) = \begin{cases} C_{[Jdt,0]}Q(u(0)) \quad \text{if } \; h \leq \epsilon \\ \left(\begin{array}{c} C_{[Jdt,0]}Q\big(u(0)\big) + \\ \sum_{j=0}^{j=J-1} RC_{[Jdt,(j+1)dt]}QF_{(j+1)dt,jdt]}RC_{[jdt,0]}Q(u(0)) \\ \sum_{j=0}^{j=J-1} RC_{[Jdt,(j+1)dt]}C_{(j+1)dt,jdt]}C_{[jdt,0]}Q(u(0)) \end{array} \right) & \text{if } \; \epsilon < h \leq \gamma \\ F_{[Jdt,0]}(u(0)) \quad \text{if } \; h > \gamma \end{cases}$$

Hybridization Charged Particle in Magnetic Mirror



$$B_x = -\frac{2Cxz^3}{a^4}$$

$$\mathrm{B_y} = -\frac{\mathrm{2Cyz^3}}{\mathrm{a^4}}$$

$$\mathrm{Bz} = \mathrm{C}\left(1 - \frac{\mathrm{z^4}}{\mathrm{a^4}}\right)$$

Gyrokinetic + Phase and Time Parallel method are the most efficient

Simple blending could be more accurate as the problem approaches stead state

*Submitted to Journal

Summary

- **Collisional Radiative**
  - Boltzmann grouping improves group representation over applied uniform distribution
  - Minimization of error, which is expected to accumulate quickly during highly-transient durations, and acceleration of method makes Boltzmann reduction a strong case for future coupled simulations
  - Adaptive integration allowed for faster simulations at larger electron temperatures
  - Sensitive to selected groups
  - Grouping reduces stiffness
  - Robust solver capable of handling, Te from 1 – 1,000 eV and 10^{16}-10^{24} particles
  - Initial work on non-Maxwellian CR has begun and early numerical issues have been addressed
- **Hybridization**
  - Shows that hybridization technique can be more computational efficient than the schemes that comprise it

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Future Work

- **Collisional Radiative Simulations**
  - Further comparisons between reduced mechanisms with QSS
  - Line identification and width assignments in conjunction with experimental spectra
  - Apply Boltzmann grouping to new CR Argon rates and test with 1D MHD Argon shock by Kapper, et.al. Future plans to extend to 2 and 3D MF
  - Rerun previous LPI test case with level grouping; laser source term, heavy-electron elastic collisions, and multi-electron energy correction and heavy energy equation (Te, Th)
- **Group selection through numerical analysis, optimization**
- **Hybridize Maxwellian CR with QSS**
- **Non-Maxwellian finite rate EEDF implementation**

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Questions?